

Journal of

Computational Physics

VOLUME 75, 1988



ACADEMIC PRESS, INC.

Harcourt Brace Jovanovich, Publishers

San Diego New York Boston

London Sydney Tokyo Toronto

Copyright © 1988 by Academic Press, Inc.
All Rights Reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (27 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1988 articles are as shown on the article title pages; if no fee code appears on the title page, the copy fee is the same as for current articles.

0021-9991/88 \$3.00

Printed by Catherine Press, Ltd., Brugge, Belgium

CONTENTS OF VOLUME 75

NUMBER 1, MARCH 1988

S. MAFÉ, J. PELLICER, AND V. M. AGUIELLA. A Numerical Approach to Ionic Transport Through Charged Membranes	1
J. M. FLÓRYAN AND CHARLES ZEMACH. Quadrature Rules for Singular Integrals with Application to Schwarz-Christoffel Mappings	15
A. CLOOT AND B. M. HERBST. Grid Resonances, Focusing, and Benjamin-Feir Instabilities in Leapfrog Time Discretizations	31
JEFFREY C. BUELL. A Mixed Finite Difference/Galerkin Method for Three-Dimensional Rayleigh-Bénard Convection	54
G. C. POMRANING. Initial and Boundary Conditions for Flux-Limited Diffusion Theory	73
JAMES G. BERRYMAN. Interpolating and Integrating Three-Point Correlation Functions on a Lattice	86
BORIS D. LUBACHEVSKY. Efficient Parallel Simulations of Dynamic Ising Spin Systems	103
ULRICH SCHUMANN AND ROLAND A. SWEET. Fast Fourier Transforms for Direct Solution of Poisson's Equation with Staggered Boundary Conditions	123
D. J. ADAMS. The Implementation of Fluid Phase Monte Carlo on the DAP	138
R. J. MACKINNON AND G. F. CAREY. Analysis of Material Interface Discontinuities and Superconvergent Fluxes in Finite Difference Theory	151
J. H. WHEALTON, G. L. CHEN, R. J. RARIDON, R. W. McGAFFEY, E. F. JAEGER, M. A. BELL, AND D. J. HOFFMAN. A 3D Analysis of Maxwell's Equations for Cavities of Arbitrary Shape	168
CLIVE TEMPERTON. A New Set of Minimum-Add Small- <i>n</i> Rotated DFT Modules	190
CLIVE TEMPERTON. A Self-sorting In-place Prime Factor Real/Half-Complex FFT Algorithm	199
SERGE GAUTHIER. A Spectral Collocation Method for Two-Dimensional Compressible Convection	217
NOTES	
W. M. PICKERING AND P. J. HARLEY. Poisson's Equation, Hexagonal Grids and FFT Methods: Periodic Boundary Conditions	236
CARLOS A. MARTIN AND GUSTAVO MONTI. Nonlinear-Multiple-Function Simultaneous Least Squares Fitting Procedure	244
LIST OF FORTHCOMING ARTICLES	
	251

GRÉTAR TRYGGVASON. Numerical Simulations of the Rayleigh-Taylor Instability	253
J. L. ANDERSON AND D. W. HOBILL. A Study of Nonlinear Radiation Damping by Matching Analytic and Numerical Solutions	283
T. PASSOT AND A. POUQUET. Hyperviscosity for Compressible Flows Using Spectral Methods	300
JOHN A. SCALES, ADAM GERSZTENKORN, AND SVEN TREITEL. Fast l_p Solution of Large, Sparse, Linear Systems: Application to Seismic Travel Time Tomography	314
M. PUOSKARI. A Method for Computing Bessel Function Integrals	334
MUSHENG WEI, GEORGE MAJDA, AND WALTER STRAUSS. Numerical Computation of the Scattering Frequencies for Acoustic Wave Equations	345
Y. CHOI, J. A. C. HUMPHREY, AND F. S. SHERMAN. Random-Vortex Simulation of Transient Wall-Driven Flow in a Rectangular Enclosure	359
H. MATSUO, Y. OHYA, K. FUJIWARA, AND H. KUDOH. Numerical Simulation of Cylindrically Converging Shock Waves	384
M. BRIO AND C. C. WU. An Upwind Differencing Scheme for the Equations of Ideal Magnetohydrodynamics	400
A. H. REIMAN AND H. S. GREENSIDE. Numerical Solution of Three-Dimensional Magnetic Differential Equations	423
SEIICHI KOSHIZUKA, YOSHIAKI OKA, SHUNSUKE KONDO, AND YASUMASA TOGO. Interpolating Matrix Method: A Finite Difference Method for Arbitrary Arrangement of Mesh Points	444
J. U. BRACKBILL. The Ringing Instability in Particle-in-Cell Calculations of Low-Speed Flow	469
NOTES	
STEVEN PRUESS. On Shooting Algorithms for Calculating Sturm-Liouville Eigenvalues	493
V. H. RANSOM AND D. L. HICKS. Hyperbolic Two-Pressure Models for Two-Phase Flow Revisited	498
LIST OF FORTHCOMING ARTICLES	
AUTHOR INDEX FOR VOLUME 75	

Journal of Computational Physics

INFORMATION FOR AUTHORS

The purpose of the *Journal of Computational Physics* is to publish articles concerning techniques developed in the solution of data handling problems and mathematical equations, both arising in the description of physical phenomena.

Manuscripts should be submitted to: The Editors, *Journal of Computational Physics*, University of California, Lawrence Livermore National Laboratory, P. O. Box 5509, L-561, Livermore, California 94550, U.S.A.

Only original papers will be considered. Manuscripts are accepted for review with the understanding that the same work has not been and will not be nor is presently submitted elsewhere, and that its submission for publication has been approved by all of the authors and by the institution where the work was carried out; further, that any person cited as a source of personal communications has approved such citation. Written authorization may be required at the Editors' discretion. Articles and any other material published in the *Journal of Computational Physics* represent the opinions of the author(s) and should not be construed to reflect the opinions of the Editors and the Publisher.

Authors submitting a manuscript do so on the understanding that if it is accepted for publication, copyright in the article, including the right to reproduce the article in all forms and media, shall be assigned exclusively to the Publisher. The Publisher will not refuse any reasonable request by the author for permission to reproduce any of his or her contributions to the journal.

Form of Manuscript. Manuscripts should be typewritten with wide margins on high quality 8.5×11 -in. bond paper, using double spacing throughout. If larger paper must be used, the text must still be within these dimensions. A minimum of three copies should be submitted; however, in order to expedite handling of manuscripts, five copies are desirable. The original of the manuscript and figures (including computer-generated data) need not be submitted until acceptance, as long as the copies are clear and reproducible. Figures and tables must be in all copies.

Each page of the manuscript should be numbered consecutively. Page 1 should contain the article title, author, and coauthor names with complete affiliation(s). At the bottom of this page should appear the subject classifications and key words (see below). Page 2 should contain a proposed running head of less than thirty-five characters. It should also contain the name and complete mailing address of the person to whom proofs are to be sent. Page 3 of full articles should contain a short abstract.

Notes. Short notes of 10 pages or less (including figures, tables, and references but excluding title pages) regarding the availability of interesting and useful new programs or tabular material will be considered for publication. Letters to the Editor commenting on articles already published in this Journal will also be considered. Neither notes nor letters should have an abstract.

With the exceptions noted below, authors should be guided by the *Style Manual*, 1978, of the American Institute of Physics.

Subject Classification. Authors are required to classify their own manuscripts using the 1980 *Mathematics Subject Classification*, reprinted from the 1978 *Mathematical Reviews Index*, pp. S27-S34, with the additional classifications listed in the January 1, 1981 issue. Authors are requested to choose at least two categories—one in numerical analysis category 65, and one other (generally a physical classification) from the categories beyond 65.

List of Symbols. If the paper is accepted for publication, it is of vital importance that the author submit a complete list of symbols. The symbols used should be identified for the typesetter **phonetically**. This list will not appear in print but is essential to avoid costly corrections in proof. The author may prepare his or her own list or use a preprinted form supplied by the Editors.

Tables. Number tables consecutively with Roman numerals. Extensive tables will be reproduced photographically and should be typed carefully in the **exact** format desired. Authors will be charged for any new photoreproductions necessitated by changes in proof. Use superscript lowercase italic letters for table footnotes, which should be typed immediately below the table. Type tables at least double-spaced, including titles and footnotes. Do not underline table titles; reserve underlining for text that is to be *italicized*.

Equations. Equations should be typewritten whenever possible and the number placed in parentheses at the right margin. Reference to equations should use the form "Eq. (3)" or simply "(3)." Superscripts and subscripts should be typed or handwritten clearly above and below the line, respectively. Use the exponent $^{1/2}$ whenever possible.

References. References should be cited in the text by a number in square brackets. Literature cited should appear on a separate page at the end of the article and should be styled and punctuated according to the standards of the American Physical Society and using standard abbreviations for journals (see *Chemical Abstracts Service Source Index*, 1985). See the following examples:

1. D. SCHNACK AND J. KILLEEN, *J. Comput. Phys.* **35**, 110 (1980).
2. I. GOHBERG, P. LANCASTER, AND L. RODMAN, *Matrix Polynomials* (Academic Press, New York, 1982), p. 54.
3. R. GROSS, M. KOYANAGI, H. SEIFERT, AND R. P. HUEBENER, in *Proceedings, 17th Int. Conf. on Low Temperature Physics, Karlsruhe, West Germany, 1984*, edited by U. Eckern *et al.* (North-Holland, Amsterdam, 1984), p. 431.

For unpublished lectures or symposia, include title of paper, name of sponsoring society in full, and date. Abbreviation of DOE Laboratory report names should follow the style of *Nuclear Science Abstracts*. Give titles of unpublished reports with "(unpublished)" following the reference. Further examples and instructions are available from the Editors.

Footnotes. Footnotes in the text should be avoided if at all possible. If they must be used, identify by superscript numbers and type together on a separate page, double-spaced.

Figures. All illustrations are to be considered as figures. Number each graph or drawing in sequence with Arabic numerals. Supply a descriptive legend for each figure. Type legends double-spaced consecutively on a separate page.

Plan figures to fit the proportion of the printed page. Use a professional lettering set on the original so that the letters and numbers are large enough and "open" enough to take a reduction of 50 to 60% without filling in the ink. Do not include background grids; however, on paper with blue lines the grid can be eliminated in the process of photoreproduction. Identify each figure in a margin with the name of the journal, author's name, and figure numbers; avoid marking the backs of figures.

Proofs. Proofs will be sent to the author with a reprint order form. Authors will be charged for alterations in excess of 10% of the cost of composition.

Reprints. Fifty reprints without covers will be provided free of charge. Additional reprints may be purchased.